

# Improved Calculation of Thermal Fission Energy <sup>☆</sup>

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## Abstract

Thermal fission energy is one of the basic parameters needed in the calculation of antineutrino flux for reactor neutrino experiments. It is useful to improve the precision of the thermal fission energy calculation for current and future reactor neutrino experiments, which are aimed at more precise determination of neutrino oscillation parameters. In this article, we give new values for thermal fission energies of some common thermal reactor fuel isotopes, with improvements on two aspects. One is more recent input data acquired from updated nuclear databases. The other, which is unprecedented, is a consideration of the production yields of fission fragments from both thermal and fast incident neutrons for each of the four main fuel isotopes. The change in calculated antineutrino flux due to the new values of thermal fission energy is about 0.33%, and the uncertainties of the new values are about 15% to 50% smaller.

*Keywords:*

energy released in fission, reactor, neutrino experiment, antineutrino flux

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## 1. Introduction

Reactor neutrino experiments have always played a critical role in the history of neutrino physics. For example, the Savannah River Experiment[1, 2] by Reines and Cowan in 1956 first detected the neutrino. The KamLAND[3] experiment confirmed neutrino oscillation and explained the solar neutrino deficit together with the SNO experiment in the first few years after 2000.

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Just before that, the CHOOZ [4] experiment determined the most stringent upper limit of the last unknown neutrino mixing angle,  $\sin^2 2\theta_{13} < 0.17$  at 90% confidence level. After this, a generation of reactor neutrino experiments made efforts to determine the value of  $\theta_{13}$ . In March of 2012, the Daya Bay collaboration[5] discovered a non-zero value for  $\sin^2 2\theta_{13}$  at a  $5\sigma$  confidence level, which has fueled discussions about the direction of neutrino physics in the foreseeable future.

The prediction of antineutrino flux and its uncertainty is an indispensable part of reactor neutrino experiments, especially absolute measurement experiments which use a single detector. Usually, the following formula is used to calculate the antineutrino flux from one reactor core:

$$S(E_\nu) = \frac{W_{th}}{\sum_i (f_i/F) E_i} \sum_i (f_i/F) S_i(E_\nu) \quad (1)$$

Where  $W_{th}$ (MeV/s) is the thermal power of the core,  $E_i$ (MeV/fission) is the energy released per fission for isotope  $i$ ,  $f_i$  is the fission rate of isotope  $i$ , and  $F$  is the sum of  $f_i$  for all isotopes. Thus,  $f_i/F$  is the fission fraction of each isotope.  $S_i(E_\nu)$  is the antineutrino energy spectrum of isotope  $i$ , which is normalized to one fission. Normally,  $W_{th}$  and  $f_i/F$  of each isotope are supplied by the nuclear power plants of the reactor neutrino experiments. This leaves  $E_i$  and  $S_i(E_\nu)$  as the two decisive parameters for the accurate calculation of antineutrino flux. In this article, we restrict our discussion to  $E_i$  only. We will explain how we improve the precision of the calculation of  $E_i$  on two aspects, and compare the new value and its error with those from predecessors.

## 2. Calculation Method of Thermal Fission Energy $E_f$

The energy release per fission  $E_f$  can be represented as the sum of the four terms[6].

$$E_f = E_{total} - \langle E_\nu \rangle - \Delta E_{\beta\gamma} + E_{nc} \quad (2)$$

Where  $E_{total}$  is the total average energy in fission from the instant at which the neutron that induces the process is absorbed to the completion of the beta decays of the product fragments and their transformation into beta-stable atoms. It includes the total kinetic energy of the fission fragments, total kinetic energy of the emitted prompt and delayed neutrons, and all kinetic energy of the emitted photons,  $\beta$  particles, and antineutrinos.  $\langle E_\nu \rangle$  is the

mean energy carried away by antineutrinos that are produced in the beta decay of fission fragments,  $\Delta E_{\beta\gamma}$  is the energy of beta electrons and photons from fission fragments that did not decay at a given instant of time.  $E_{nc}$  is the energy released in neutron capture (without fission) by various materials of the reactor core.

The energy from the fission process which remains in the reactor core and is transformed into heat can be defined as effective fission energy  $E_{eff}$ :

$$E_{eff} = E_{total} - \langle E_\nu \rangle - \Delta E_{\beta\gamma} \quad (3)$$

then, relation(2) can be recast into form

$$E_f = E_{eff} + E_{nc} \quad (4)$$

If  $E_{total}$  is calculated by applying the energy-conservation law, and then  $\langle E_\nu \rangle$ ,  $\Delta E_{\beta\gamma}$ , and  $E_{nc}$  are calculated, we can obtain the value of thermal fission energy  $E_f$ .

### 3. Calculation Procedures and Results

#### 3.1. Total fission energy $E_{total}$

Total fission energy  $E_{total}$  can be obtained by directly applying the energy-conservation law. The formula is

$$M(A_0, Z_0) + M_n = \sum y_A M(A, Z_A) + \nu M_n + E_{total} \quad (5)$$

where  $M(A_0, Z_0)$  is the atomic mass of the isotope undergoing fission;  $A_0$  and  $Z_0$  are its mass and charge numbers respectively;  $M_n$  is the neutron mass; summation is performed over the mass number  $A$  of beta-stable fission products;  $M(A, Z_A)$  is the atomic mass of these products, and  $y_A$  are their yields,  $\sum y_A = 2$ . The values of  $A$  are from 66 through 172.  $\nu$  is the mean total number of the prompt and delayed fission neutrons. Using the condition that the number of nucleons is conserved in the fission process and introducing the mass excess for atoms  $m(A, Z)$ , equation (5) can be rewritten as:

$$E_{total} = m(A_0, Z_0) - \sum y_A m(A, Z_A) - (\nu - 1)m_n \quad (6)$$

where  $m(A, Z) = M(A, Z) - Am_0$  ( $m_0$  is an atomic mass unit) and  $m_n = M_n - m_0 = 8.07131710 \pm 0.00000053$  MeV is the neutron mass excess. Thus,

Table 1: Fission ratios of  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$  and  $^{241}\text{Pu}$  induced by thermal and fast neutrons

Fissile isotopes	Thermal neutron	Fast neutron
$^{235}\text{U}$	76.82%	23.18%
$^{238}\text{U}$	0.00%	100.00%
$^{239}\text{Pu}$	90.25%	9.75%
$^{241}\text{Pu}$	83.11%	16.89%

$m(A_0, Z_0)$  and  $m(A, Z_A)$  are the mass excess of the isotope undergoing fission and of the fission products, respectively. These values can be obtained from the mass excess evaluation in ATE2003[7]. Mass excess  $m(A, Z_A)$  for beta-stable atoms is shown in Fig.1.

According to the INDC[8] and other nuclear databases[9], for each isotope, the yield  $y_A$  of each fission fragment in thermal neutron induced fission is different from that of the same fission fragment in fast neutron induced fission. Up to now, calculations have simply treated all fissions of  $^{238}\text{U}$  as being induced by fast neutrons and all fissions of  $^{235}\text{U}$ ,  $^{239}\text{Pu}$ , and  $^{241}\text{Pu}$  as being induced by thermal neutrons. However, reactor core simulation data from the Daya Bay Nuclear Power Plant shows that some fissions of  $^{235}\text{U}$ ,  $^{239}\text{Pu}$ , and  $^{241}\text{Pu}$  are also induced from fast neutrons. The average fission ratios of the four isotopes from thermal neutrons and fast neutrons during reactor stable running time are shown in table 1. To include the fission processes from both thermal neutrons and fast neutrons, we use the ratios in table 1 to calculate the average yield  $y_A$  for each fission fragment of each isotope. The results of  $y_A$  are shown in Fig.2. The mean total number of the emitted prompt and delayed fission neutrons  $\nu$  are also obtained from the INDC database[8].

With information from the latest nuclear databases, including mass excess, fission yield  $y_A$ , and mean fission neutron number, the total fission energy  $E_{total}$  of each isotope is obtained by taking into account both thermal and fast incident neutrons. The parameter values from the latest databases and  $E_{total}$  results are given in Table 2.

### 3.2. Average antineutrino energy $\langle E_\nu \rangle$ , and $\Delta E_{\beta\gamma}$

To estimate the average energy of antineutrinos from the fission fragments of  $^{235}\text{U}$ ,  $^{239}\text{Pu}$  and  $^{241}\text{Pu}$ , we use the beta-to-antineutrino conversion spectra

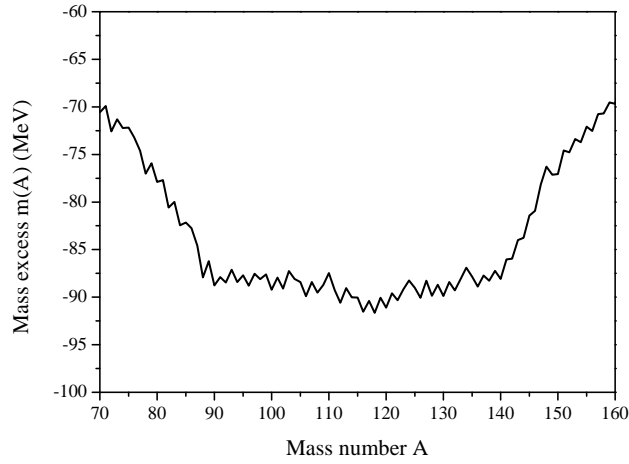


Fig. 1: Mass excess  $m(A, Z_A)$  for beta-stable atoms as a function of the mass number  $A$

Table 2: Parameters and  $E_{total}$  of  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$  and  $^{241}\text{Pu}$

Fissile isotopes	Mass excess		Fission		
	$m(A_0, Z_0)$	$y_A m(A, Z_A)$	neutrons $\nu$	$(\nu-1)m_n$	$E_{total}$
$^{235}\text{U}$	$40.9205 \pm 0.0018$	$-173.859 \pm 0.058$	$2.4355 \pm 0.0023$	11.586	$203.19 \pm 0.06$
$^{238}\text{U}$	$47.3089 \pm 0.0019$	$-173.687 \pm 0.058$	$2.8190 \pm 0.0200$	14.682	$206.32 \pm 0.06$
$^{239}\text{Pu}$	$48.5899 \pm 0.0018$	$-174.196 \pm 0.060$	$2.8836 \pm 0.0047$	15.203	$207.58 \pm 0.06$
$^{241}\text{Pu}$	$52.9568 \pm 0.0018$	$-174.100 \pm 0.065$	$2.9479 \pm 0.0055$	15.722	$211.33 \pm 0.07$

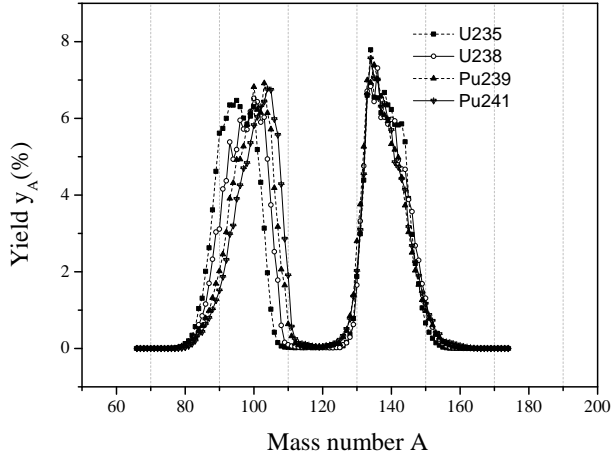


Fig. 2: Total yield  $y_A$  of beta-stable fragments originally from the fission of uranium and plutonium isotopes

of the Laue-Langevin Institute (ILL) [10, 11, 12]. The errors of these spectra are from ILL beta spectra measurements and ILL beta-to-antineutrino conversion method[10, 11]. In the case of  $^{238}\text{U}$ , we use the theoretical  $\bar{\nu}_e$  spectrum from P. Vogel, et al. [13], where the errors are theoretically estimated. We calculate non-equilibrium corrections and apply them to the ILL spectra.

To determine  $\langle E_\nu \rangle$  of each isotope, the function  $y = \exp(B_0 + B_1x + B_2x^2)$  is used to fit each spectrum, which are all limited to neutrino energies above 1.5 MeV. In the function,  $y$  is the neutrino number per fission per MeV,  $x$  is the neutrino energy, and  $B_0$ ,  $B_1$  and  $B_2$  are fitting parameters. Fitting results are shown in Fig.3. The  $\chi^2/dof$  of the fits to the ILL spectra are all close to one, which shows that the function can describe the antineutrino spectra very well. The  $\chi^2/dof$  of the  $^{238}\text{U}$  spectrum is closer to zero because the spectrum is from theoretical calculation. In addition, the estimated errors of the spectrum are larger than those of the ILL spectra on average, which also contributes to the small  $\chi^2/dof$  value. Fitting parameters are summarized in Table 3. The fits are used to smoothly extrapolate to energies below 1.5 MeV.

The average energy carried by antineutrinos  $\langle E_\nu \rangle$  is shown in Table 4. The results are consistent with those in reference [6]. The uncertainties

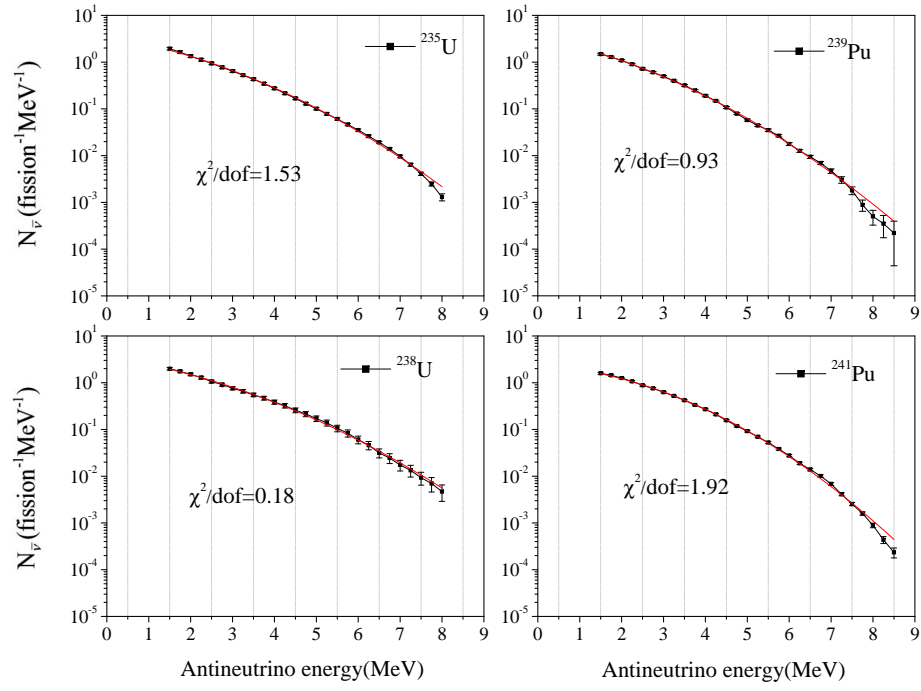


Fig. 3: Reactor antineutrino spectra of  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$  and  $^{241}\text{Pu}$

obtained by our own fitting are similar, but little smaller.

Table 3: Values of the fitting parameters

Parameter	$^{235}\text{U}$	$^{238}\text{U}$	$^{239}\text{Pu}$	$^{241}\text{Pu}$
$B_0$	1.25636	1.26119	1.20114	0.87170
$B_1$	-0.33897	-0.30588	-0.40981	-0.13055
$B_2$	-0.007309	-0.06253	-0.07690	-0.10355

Table 4: Average energy carried away by antineutrinos

Fissile isotopes	$\langle E_\nu \rangle$ (MeV)	[6] (MeV)
$^{235}\text{U}$	$9.16 \pm 0.32$	$9.07 \pm 0.32$
$^{238}\text{U}$	$10.97 \pm 0.45$	$11.00 \pm 0.80$
$^{239}\text{Pu}$	$7.12 \pm 0.13$	$7.22 \pm 0.27$
$^{241}\text{Pu}$	$8.20 \pm 0.20$	$8.71 \pm 0.30$

The kinetic energies of  $\beta$  particles and photons from the complete beta decay of fission fragments are part of the total fission energy,  $E_{total}$ . However, at the instant of observation, the decay processes of some long-life isotopes have not yet completed. The correction of  $\Delta E_{\beta\gamma}$  is used to subtract the kinetic energies of  $\beta$  particles and gammas which have not been emitted. Values for  $\Delta E_{\beta\gamma}$  are borrowed from [6] as shown in Table 5. These values correspond to a fuel irradiation time in the middle of the standard operating period of a pressurized water reactor.

Table 5: Energy  $\Delta E_{\beta\gamma}$

Fissile isotopes	$\Delta E_{\beta\gamma}$ (MeV)
$^{235}\text{U}$	$0.35 \pm 0.02$
$^{238}\text{U}$	$0.33 \pm 0.03$
$^{239}\text{Pu}$	$0.30 \pm 0.02$
$^{241}\text{Pu}$	$0.29 \pm 0.03$



### 3.3. Energy released in neutron capture $E_{nc}$

In addition to the energy released directly in the fission process, some energy is released in neutron capture upon reactor materials. The total amount of this energy depends on the composition of the reactor materials and the probability of neutron absorption on these materials, therefore it also varies with fuel burning time. In the middle of the reactor operating period, the energy from neutron capture processes  $E_{nc}$  which converts into thermal energy in fuel isotope  $i$  can be described as:

$$E_{nc} = (\bar{\nu}_i - 1)\bar{Q} \quad (7)$$

where  $\bar{Q}$  is the mean energy released per capture and  $\bar{\nu}_i$  is the average number of emitted neutrons per fission. In reference[14], a  $\bar{Q}$  of  $6.1 \pm 0.3$  MeV is given by simply considering a wide range of reactor material compositions. In reference [6], the probabilities of the absorption of neutrons by various materials, and the time evaluations of fuels during burn-up periods are both considered. The average value of  $5.97 \pm 0.15$  MeV per neutron capture is given for the middle of the reactor operation period. Its variation within the time interval from one day to the end of the operating period is about 0.55 MeV. In this paper, we use the  $\bar{Q}$  value from reference [6] and  $\bar{\nu}_i$  from INDC, which was mentioned earlier for the calculation of  $E_{total}$ . The results of  $E_{nc}$  are shown in Table 6.

Table 6: Neutron capture released energy  $E_{nc}$

Fissile isotopes	$E_{nc}$ (MeV)
$^{235}\text{U}$	$8.57 \pm 0.22$
$^{238}\text{U}$	$10.86 \pm 0.30$
$^{239}\text{Pu}$	$11.25 \pm 0.28$
$^{241}\text{Pu}$	$11.63 \pm 0.29$

### 3.4. Energy release per fission

The energy release per fission is required for reactor antineutrino flux calculations, and is usually defined without the kinetic energy of the incident and emitted neutrons[6, 14]. However, in the WIMS-D formatted libraries[15] and reference [16], the energy release per fission includes the contributions

from the kinetic energy of incident neutrons and from the decay of the capture products:

$$E_f = E_{eff} + E_{nc} + E_{in} \quad (8)$$

where  $E_{in}$  is the kinetic energy of incident neutrons. For one isotope, at each step of its fission chain, an amount of energy from the emitted fission neutrons has to be used as the incident neutron energy for next step in the fission chain. Therefore, the amount energy of  $E_{in}$  can not transform into heat until the end of the fission chain. From the view of energy conservation, at the end of the fission chain,  $E_f = E_{eff} + E_{nc} + E_{in}$ . However, as long as the fission chain has not reached its end,  $E_{in}$  has not converted into heat, and therefore has not contributed to the reactor thermal power. Thus,  $E_f$  should be equal to  $(E_{eff} + E_{nc})$ . Our calculations of  $E_f$  without  $E_{in}$ , and of  $E_{eff}$  are shown in Table 7, along with  $E_f$  from reference[6]. For  $^{239}\text{Pu}$ , the  $E_f$  directly stated in reference[6] is 209.99 MeV, which should be the sum of  $E_{eff}$  and  $E_{nc}$ . According to the values of  $E_{eff}$  and  $E_{nc}$  in the same reference,  $E_f$  of  $^{239}\text{Pu}$  should be 210.99 MeV. Thus, we list 210.99 MeV in table 7. As one can see in the table, the new  $E_f$  values are consistent with those in reference [6] within errors, but the new errors are about 15% to 50% smaller. The contributions to the improved errors of  $E_f$  are from the calculations of  $E_{total}$  and  $< E_\nu >$ .

Table 7: Energy release per fission

Fissile isotopes	$E_{eff}$ (MeV)	$E_f$ [6] (MeV)	$E_f$ (MeV)
$^{235}\text{U}$	$193.68 \pm 0.33$	$201.92 \pm 0.46$	$202.25 \pm 0.39$
$^{238}\text{U}$	$195.01 \pm 0.46$	$205.52 \pm 0.96$	$205.87 \pm 0.55$
$^{239}\text{Pu}$	$200.16 \pm 0.14$	$210.99 \pm 0.60$	$211.41 \pm 0.32$
$^{241}\text{Pu}$	$202.84 \pm 0.21$	$213.60 \pm 0.65$	$214.47 \pm 0.36$

#### 4. Impact on the Antineutrino Flux

To quantify the slight effect of the new values for energy per fission on antineutrino flux expectation in a reactor neutrino experiment, we use reactor data from the Daya Bay experiment to calculate the expected average weekly antineutrino flux of the eight antineutrino detectors. The flux obtained with

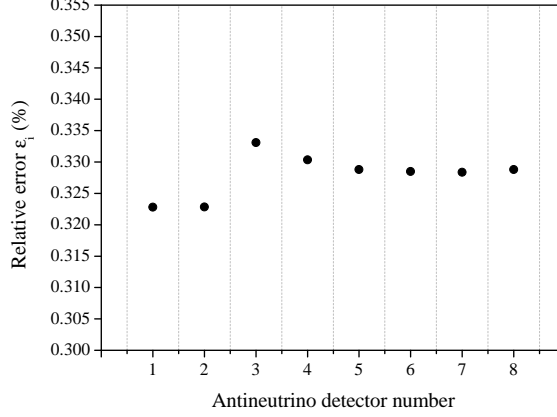


Fig. 4: Change of average weekly antineutrino flux with the input of old and new values of thermal fission energy

the input of our new thermal fission energy values is denoted as  $\phi_i$ , and that obtained with the values in reference [6] is denoted as  $\phi'_i$ . We define the relative error  $\varepsilon_i$  as

$$\varepsilon_i = |\phi'_i - \phi_i|/\phi_i \quad (9)$$

where  $i$  is the antineutrino detector number. The relative error of the weekly average antineutrino flux detected at each detector  $\varepsilon_i$  is shown in Fig. 4. The first two antineutrino detectors are at one near experimental site, called the Daya Bay site. The third and forth detectors are located at the other near site, called the Ling Ao site. The remaining four detectors are at the far site. Each detector receives antineutrinos from three reactor pairs. Due to the differences in fission fractions of isotopes between different reactor cores and the differences in baselines between detectors and reactors, the relative error varies among detectors, but they are all around 0.33%. The neutrino flux calculated with the new values is a little smaller because of a larger average energy release per fission.

## 5. Conclusion

To improve the precision of the calculation of thermal fission energy, we have employed the most recent data from nuclear databases, such as mass

excess, yield of fission fragments, and average fission neutron yields. When we apply the yield values to fission fragments, we consider the thermal and fast neutron induced fissions separately, weight them and then sum them together. These two considerations help to reduce the uncertainties of  $E_{total}$  by up to 50% compared to those given by Kopeikin[6]. Among the three other components,  $\langle E_\nu \rangle$ ,  $\Delta E_{\beta\gamma}$ , and  $E_{nc}$ ,  $\Delta E_{\beta\gamma}$  is imported from reference[6], the calculation of  $E_{nc}$  uses data of average fission neutron yield from the INDC database[8], and the estimate of  $\langle E_\nu \rangle$  is from our own fitting, which has similar but smaller uncertainties. Adding the four components together, we obtain the final thermal fission energies for  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$  and  $^{241}\text{Pu}$ . They are consistent with Kopeikin's results[6], with an improvement in uncertainty of about 15% to 50%. The impact of the new values to the expected antineutrino flux is at the level of 0.3%. We also noticed that the differences in fission energy values between reference[6, 14] and WIMSD formatted libraries[15] and reference [16] are from different treatment of incident neutron kinetic energy  $E_{in}$ . Considering that the incident neutron kinetic energy is used to propagate the fission chain and will not convert into reactor heat until the end of the fission chain, we do not include the incident neutron kinetic energy into the thermal fission energy when calculating antineutrino flux.

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## References

- [1] C. L. Cowan Jr., F. Reines, F. B. Harrison et al. Science. 1956, **124**: 103–104.
- [2] F. Reines, C.L.Cowan, Jr. Nature, 1956, **178**: 446–449.
- [3] T. Araki et al., Phys. Rev. Lett.2005, **94**: 081801.
- [4] M. Apollonio et al. Eur. Phys. J. 2003, **C27**: 331–374

- [5] F.P. An, et al., Daya Bay Collaboration, Observation of electronCan-  
tineutrino dis-appearance at Daya Bay, Phys. Rev. Lett. 2012, **108**:  
171803
- [6] V.Kopeikin, L.Mikaelyan,V.Sinev, Reactor as a source of antineutrinos:  
thermal fission energy, arXiv:hep-ph/0410100v1 7 Oct 2004
- [7] G.Audi, A.H.Wapstra and C.Thibault, The Ame2003 atomic mass eval-  
uation (II), Nuclear Physics A 729, 337-676, December 22, 2003.
- [8] A.L.Nichols, D.L.Aldama, M.VerPELLI. HANDBOOK OF NU-  
CLEAR DATA FOR SAFEGUARDS: ADDENDUM, AUGUST  
2008, INDC(NDS)-0534: 77-88
- [9] M. Herman and A. Trkov ENDF-6 Formats Manual, Data Formats  
and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and  
ENDF/B-VII, Written by the Members of the Cross Sections Evaluation  
Working Group, CSEWG Document ENDF-102, Report BNL-90365-  
2009.
- [10] K. Schreckenbach, G. Colvin, W. Gelletly, et.al. Phys.Lett. B, 1985, 160:  
325-330
- [11] A.A. Hahn, K. Schreckenbach, G. Colvin, et.al. Phys.Lett. B, 1989,  
218:365-368
- [12] F. Von Feilitzsch, A.A. Hahn, K. Schreckenbach. Phys.Lett. B, 1982,  
118:162-166
- [13] P. Vogel, G. K. Schenter, F. M. Mann, and R. E. Schenter, Phys. Rev.  
C, 1981, 24:1543
- [14] M.F.James, Journal of Nuclear Energy, 1969, Vol. 23:517-536
- [15] IAEA, WIMS-D library update : final report of a coordinated research  
project. -Vienna : International Atomic Energy Agency, 2007, 20:21
- [16] Andreja Persic, Andrej Trkov, Nuclear Energy in Central Europe '99,  
Portoroz, Slovenia, 6 to 9 september, 1999